

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030723\
 Data File : BF132686.D
 Acq On : 07 Mar 2023 19:38
 Operator : CG\JU
 Sample : 01825-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HH-TP4-0306

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132686.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.228	444	449	459	rVB	1362771	1787336	42.55%	4.651%
2	5.616	511	515	519	rBV	3652902	3652225	86.94%	9.503%
3	6.616	680	685	688	rBV	3591200	3666048	87.27%	9.539%
4	6.987	744	748	751	rBV	1374925	1108216	26.38%	2.884%
5	7.551	839	844	847	rBV	2776845	2478114	58.99%	6.448%
6	8.269	963	966	970	rBV	1569287	1432409	34.10%	3.727%
7	9.345	1145	1149	1153	rBV	4558007	4200749	100.00%	10.931%
8	10.033	1262	1266	1269	rBV	2005728	1650075	39.28%	4.294%
9	10.745	1380	1387	1391	rBV	228135	192122	4.57%	0.500%
10	10.828	1397	1401	1404	rBV	3177264	2774318	66.04%	7.219%
11	11.527	1516	1520	1523	rBV	1992176	1757574	41.84%	4.573%
12	11.551	1523	1524	1528	rVV	237187	136690	3.25%	0.356%
13	11.604	1528	1533	1534	rVV2	50739	61785	1.47%	0.161%
14	11.622	1534	1536	1541	rVB	106015	92291	2.20%	0.240%
15	11.869	1573	1578	1581	rBV2	87906	95761	2.28%	0.249%
16	11.933	1586	1589	1592	rBV2	57267	52126	1.24%	0.136%
17	12.039	1604	1607	1616	rVV4	473385	534326	12.72%	1.390%
18	12.110	1616	1619	1621	rVV	52955	45520	1.08%	0.118%
19	12.139	1621	1624	1627	rVV2	126735	138884	3.31%	0.361%
20	12.174	1627	1630	1632	rVV2	74640	81146	1.93%	0.211%
21	12.204	1632	1635	1639	rVB3	102292	98049	2.33%	0.255%
22	12.292	1647	1650	1651	rBV	72766	57908	1.38%	0.151%
23	12.398	1665	1668	1669	rBV	60013	48559	1.16%	0.126%
24	12.416	1669	1671	1674	rVB	160705	137609	3.28%	0.358%
25	12.480	1679	1682	1685	rVB	68791	61529	1.46%	0.160%
26	12.580	1694	1699	1701	rBV3	63442	95960	2.28%	0.250%
27	12.610	1701	1704	1707	rVV	166221	165098	3.93%	0.430%
28	12.639	1707	1709	1711	rVV	125584	120519	2.87%	0.314%
29	12.669	1711	1714	1719	rVB2	273072	277324	6.60%	0.722%
30	12.751	1724	1728	1732	rBV	713487	645010	15.35%	1.678%
31	12.798	1732	1736	1740	rVV2	158623	243109	5.79%	0.633%
32	12.833	1740	1742	1746	rVV3	130958	141776	3.38%	0.369%
33	12.874	1746	1749	1752	rVB3	51839	51384	1.22%	0.134%
34	12.980	1764	1767	1773	rVB	666973	600169	14.29%	1.562%
35	13.121	1786	1791	1794	rBV	4279472	3916027	93.22%	10.190%
36	13.198	1800	1804	1807	rBV3	44899	74493	1.77%	0.194%

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37	13.286	1815	1819	1820	rBV3	52459	58490	1.39%	0.152%
38	13.310	1820	1823	1825	rVV	82686	95258	2.27%	0.248%
39	13.339	1825	1828	1832	rVB2	86599	83636	1.99%	0.218%
40	13.416	1837	1841	1843	rBV2	68982	78745	1.87%	0.205%
41	13.545	1859	1863	1868	rVB3	88080	98179	2.34%	0.255%
42	13.821	1907	1910	1914	rVB	62445	64864	1.54%	0.169%
43	13.933	1925	1929	1932	rBV2	57473	81585	1.94%	0.212%
44	14.010	1936	1942	1953	rVV5	278866	509784	12.14%	1.327%
45	14.145	1962	1965	1967	rBV	93736	78289	1.86%	0.204%
46	14.186	1967	1972	1975	rVV2	1305197	1436143	34.19%	3.737%
47	14.210	1975	1976	1984	rVB	298226	243004	5.78%	0.632%
48	14.574	2036	2038	2041	rVB	75079	62226	1.48%	0.162%
49	15.039	2114	2117	2121	rVB	525622	560786	13.35%	1.459%
50	15.268	2152	2156	2160	rBV	264194	417163	9.93%	1.085%
51	15.598	2208	2212	2218	rVB	152131	180009	4.29%	0.468%
52	15.663	2219	2223	2228	rBV	233186	278838	6.64%	0.726%
53	15.733	2230	2235	2239	rBV2	796340	1056602	25.15%	2.749%
54	17.315	2499	2504	2512	rBV2	97979	201270	4.79%	0.524%
55	17.798	2582	2586	2598	rVB	81480	173486	4.13%	0.451%

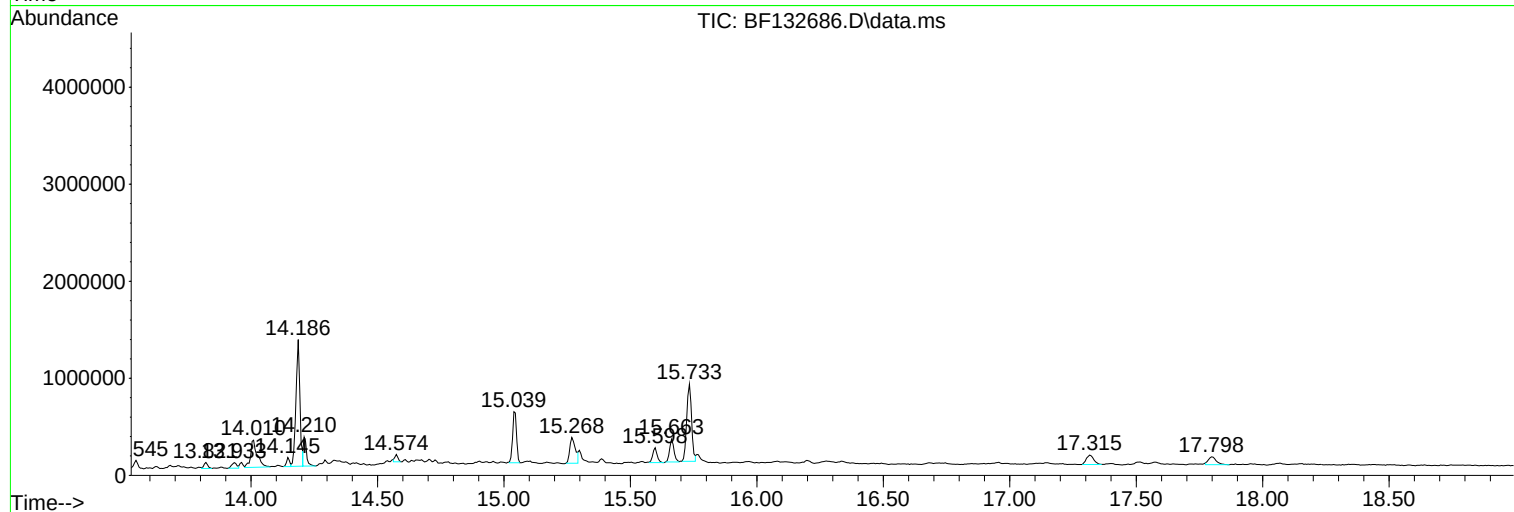
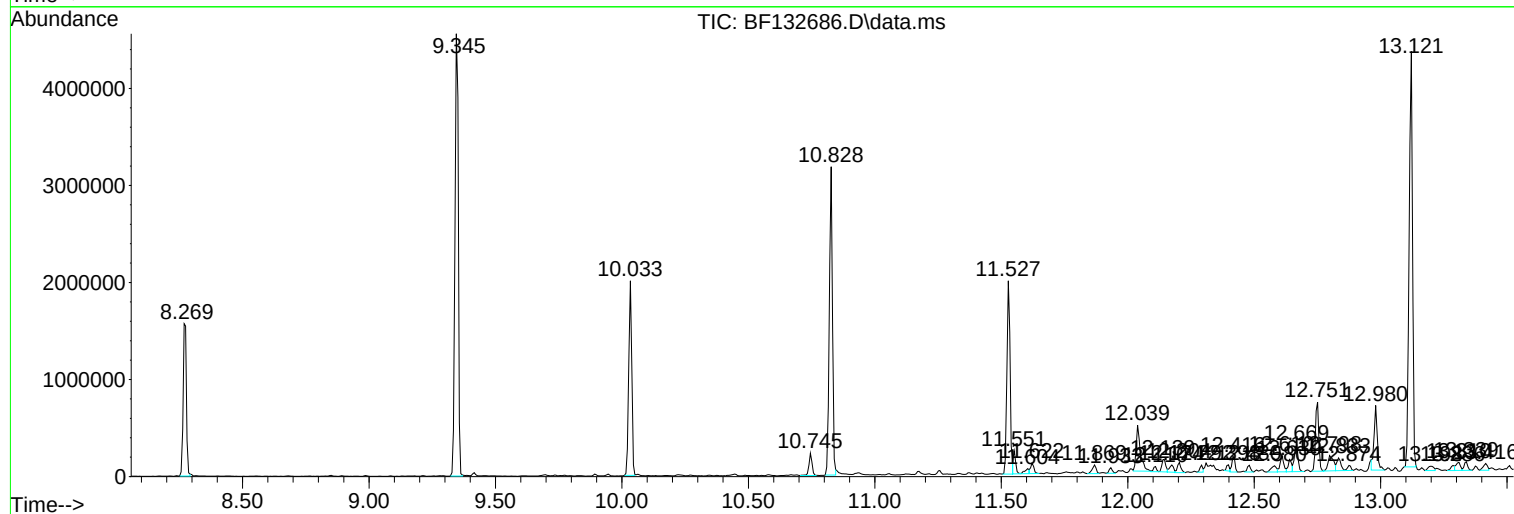
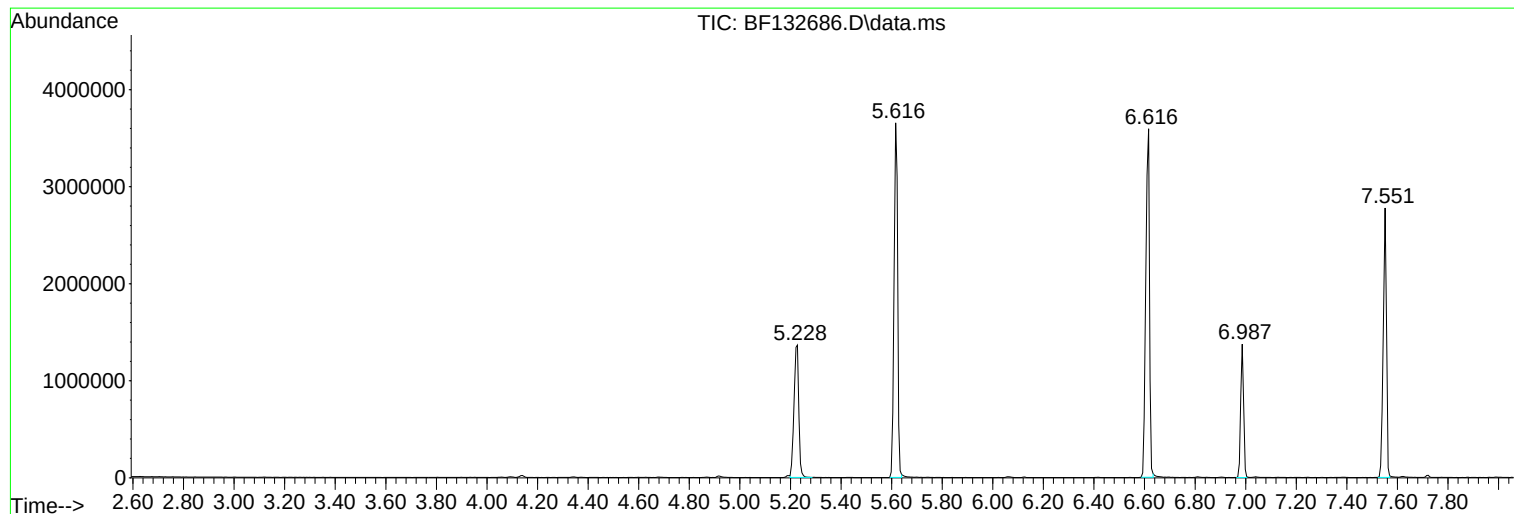
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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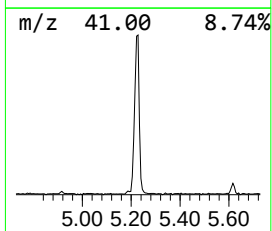
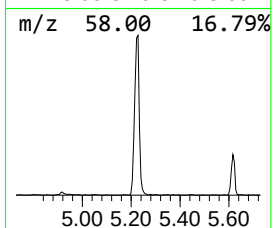
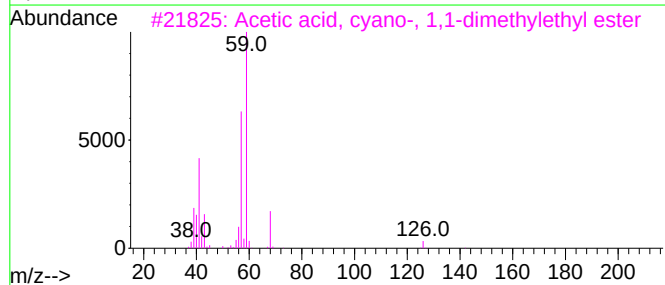
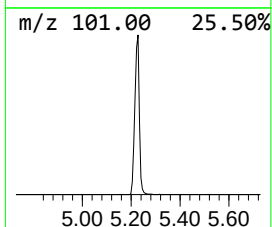
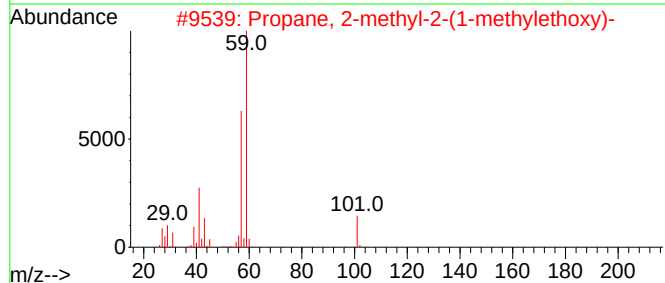
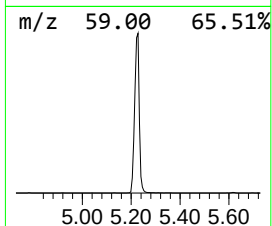
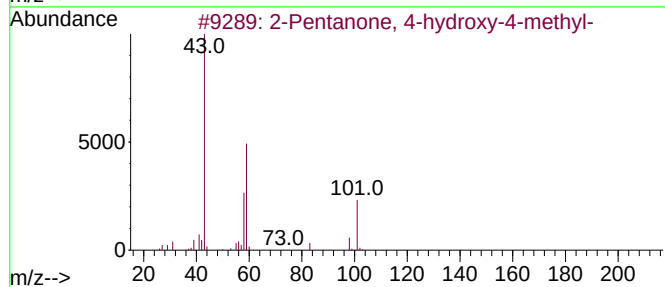
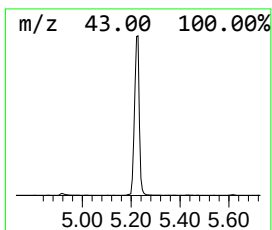
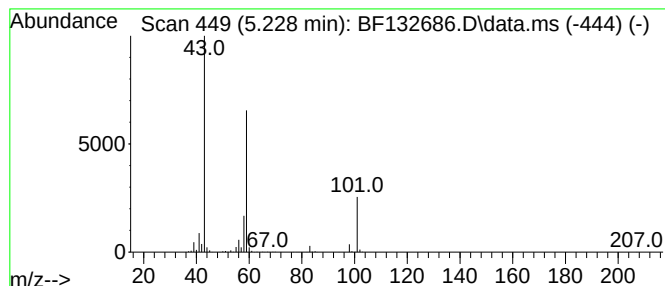
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.228	32.26 ng	1787340	1,4-Dichlorobenzene-d4	6.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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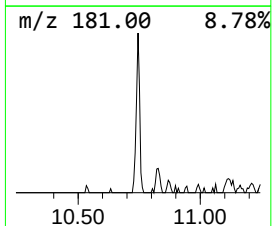
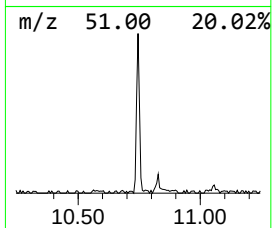
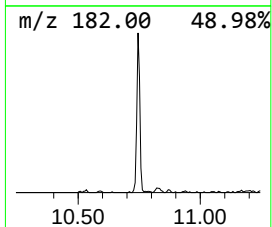
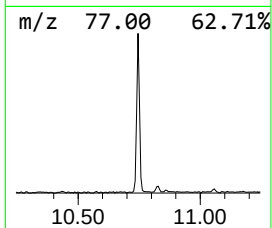
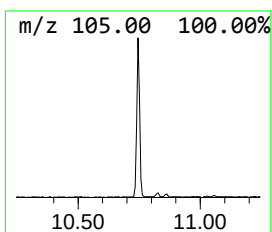
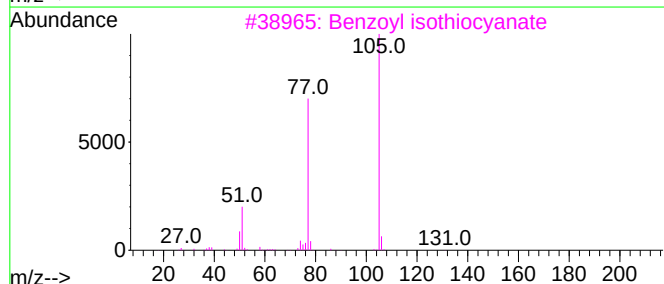
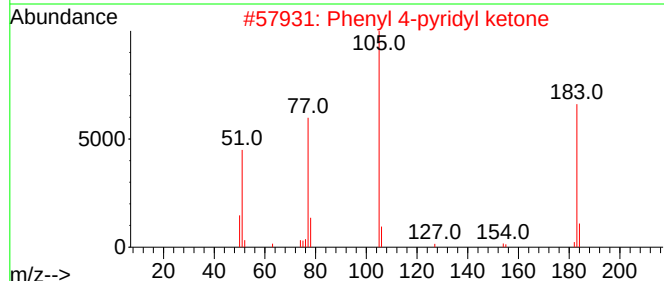
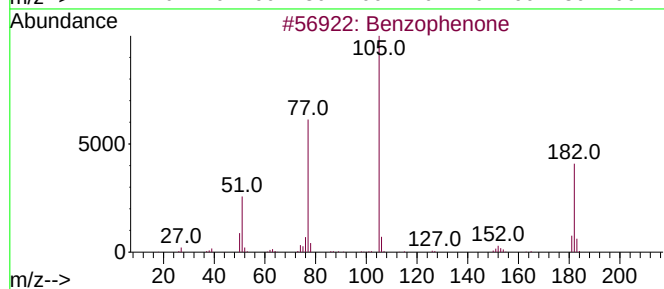
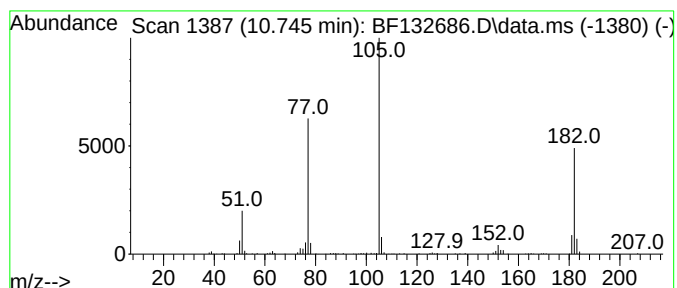
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	2.33 ng	192122	Acenaphthene-d10	10.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



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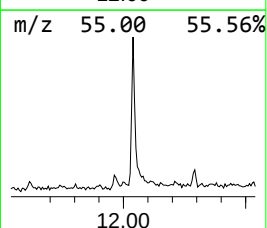
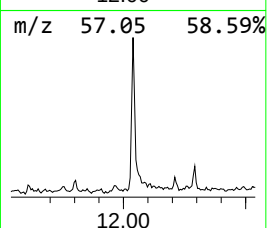
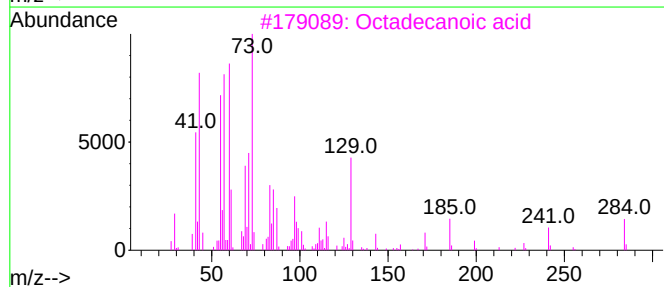
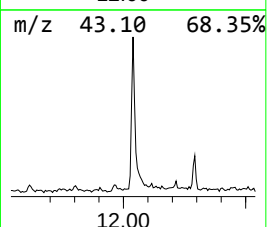
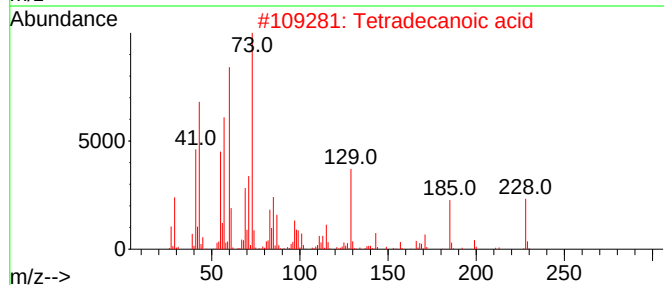
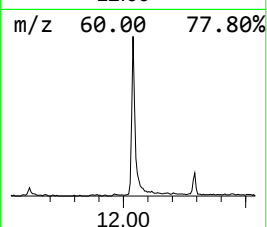
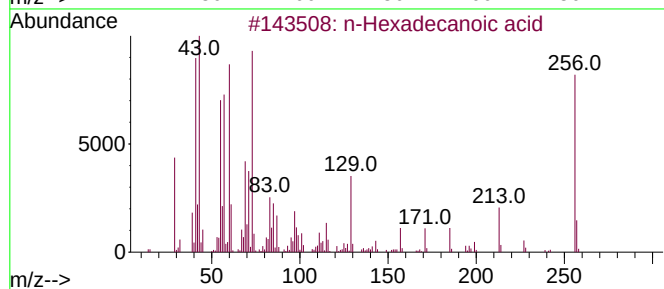
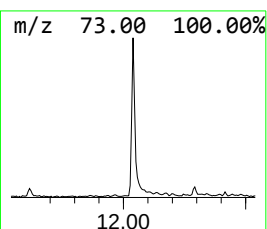
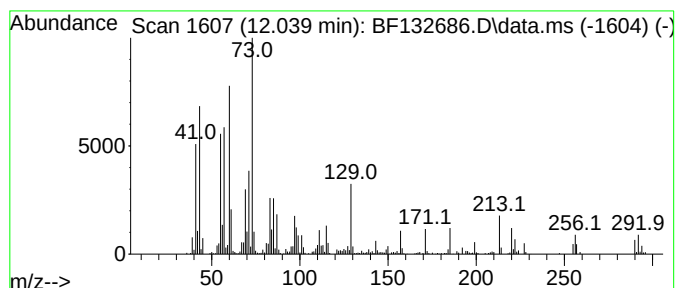
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	6.08 ng	534326	Phenanthrene-d10	11.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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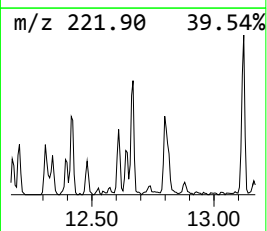
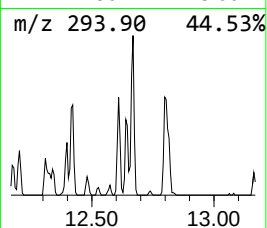
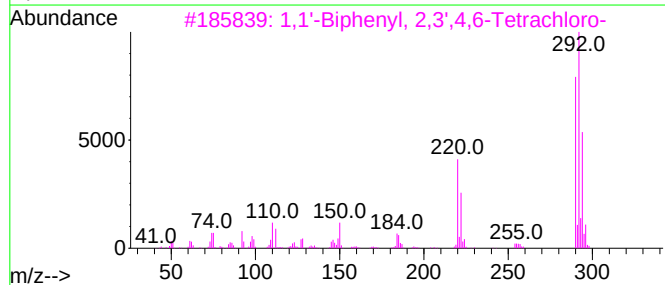
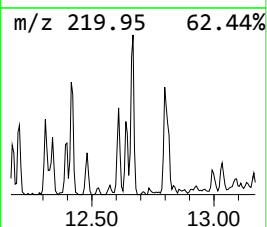
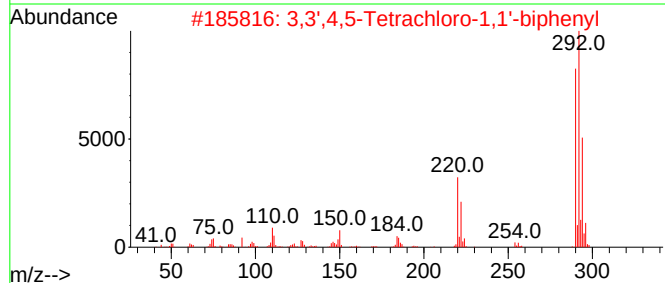
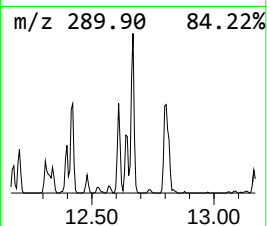
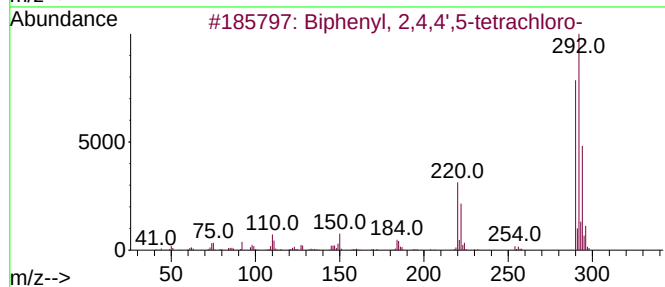
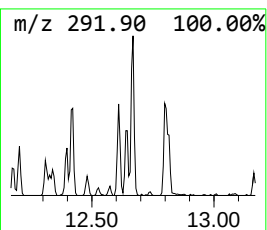
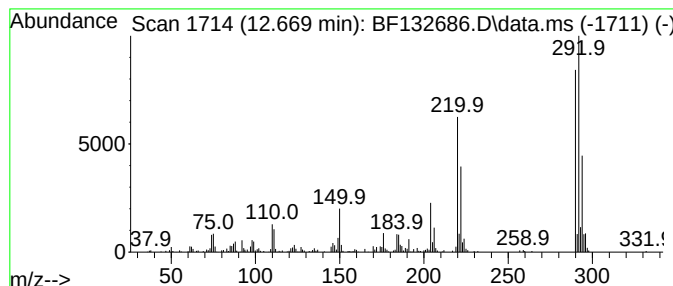
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Peak Number 4 Biphenyl, 2,4,4',5-tetrachl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	3.16 ng	277324	Phenanthrene-d10	11.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl, 2,4,4',5-tetrachloro-	290	C12H6Cl4	032690-93-0	99
2			3,3',4,5-Tetrachloro-1,1'-biphenyl	290	C12H6Cl4	070362-49-1	99
3			1,1'-Biphenyl, 2,3',4,6-Tetrachl...	290	C12H6Cl4	060233-24-1	99
4			1,1'-Biphenyl, 2,2',4,4'-tetrach...	290	C12H6Cl4	002437-79-8	99
5			1,1'-Biphenyl, 3,3',4,5'-tetrach...	290	C12H6Cl4	041464-48-6	99



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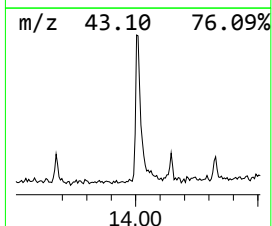
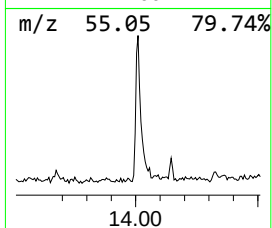
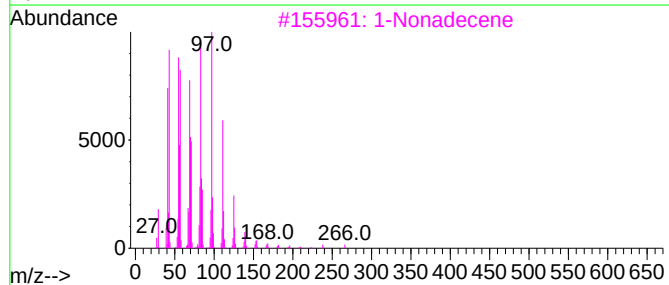
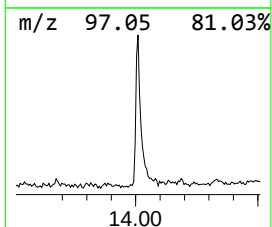
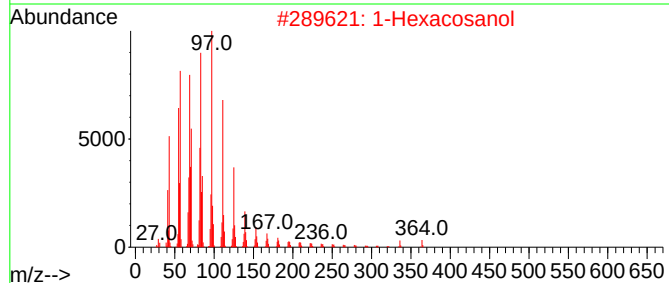
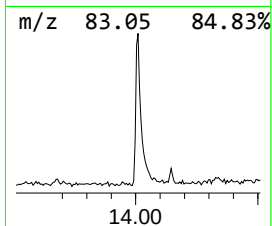
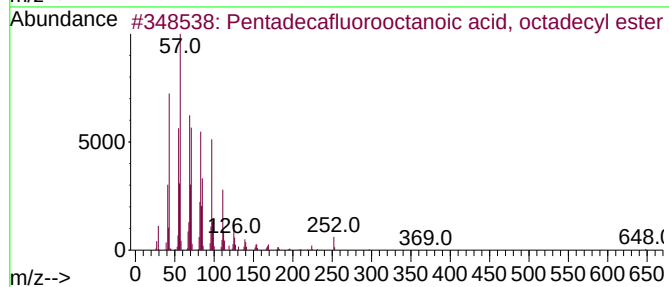
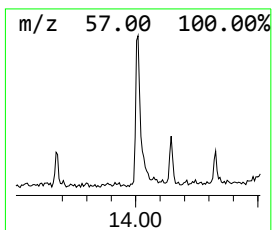
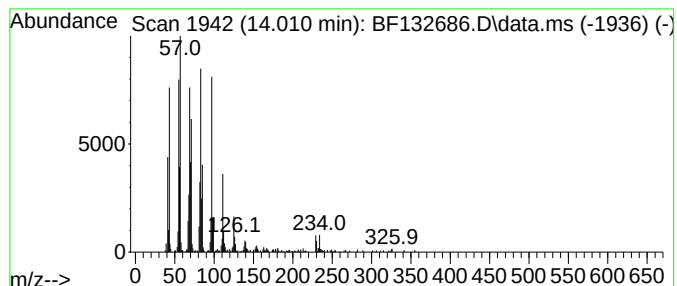
Instrument :
BNA_F
ClientSampleId :
HH-TP4-0306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.010	7.10 ng	509784	Chrysene-d12	14.186	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, octadecyl ester	666	C26H37F15O2	1000406-04-8	94
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5	Dichloroacetic acid, heptadecyl ester	366	C19H36Cl2O2	1000282-98-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030723\
Data File : BF132686.D
Acq On : 07 Mar 2023 19:38
Operator : CG\JU
Sample : 01825-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-TP4-0306

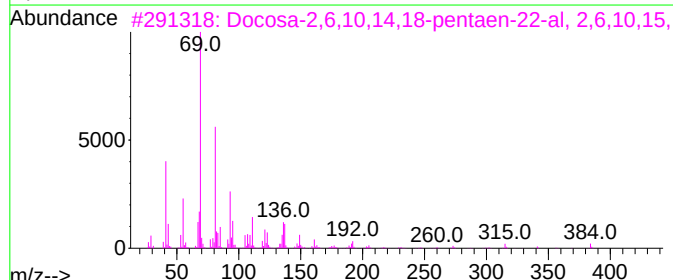
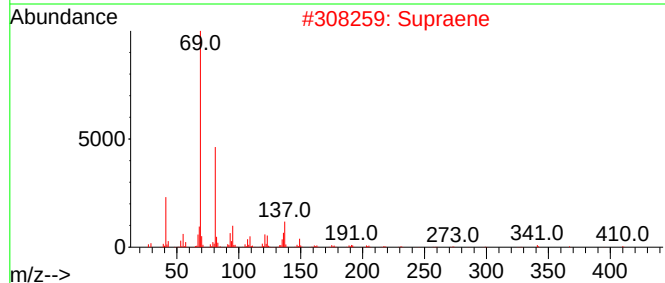
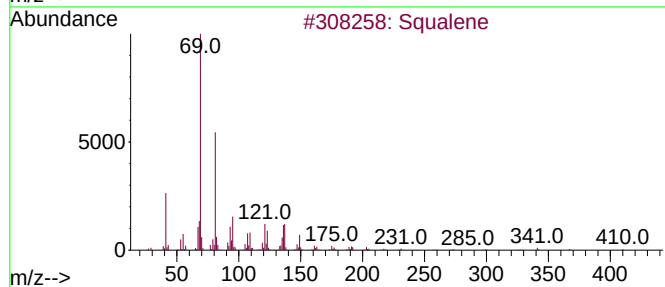
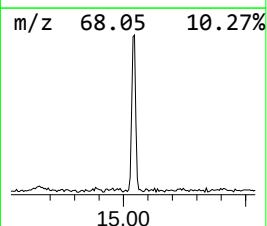
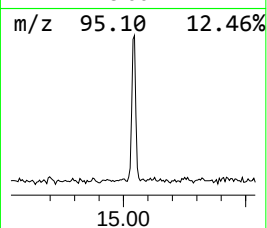
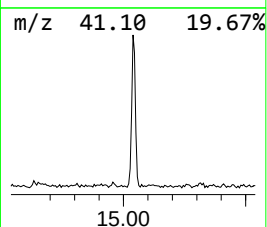
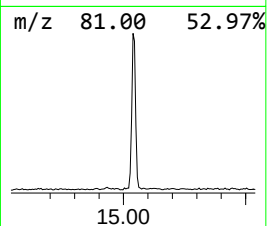
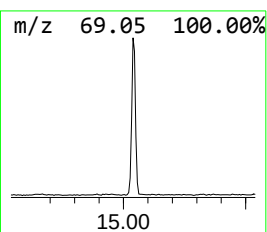
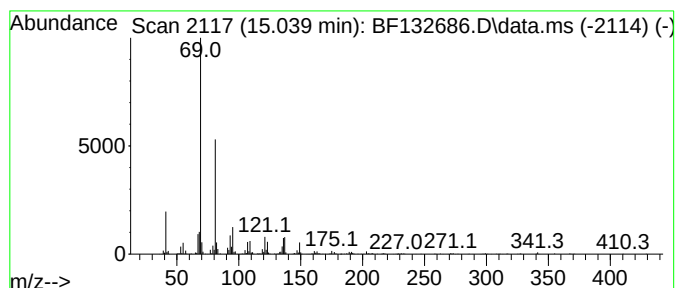
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	10.61 ng	560786	Perylene-d12	15.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	97
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5			Farnesol isomer a	222	C15H26O	1000108-92-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030723\
Data File : BF132686.D
Acq On : 07 Mar 2023 19:38
Operator : CG\JU
Sample : 01825-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-TP4-0306

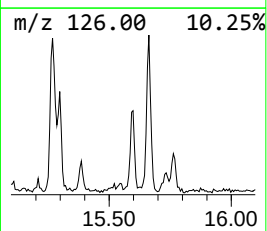
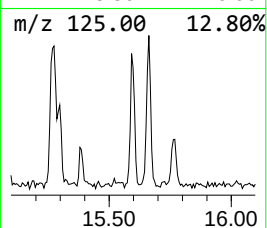
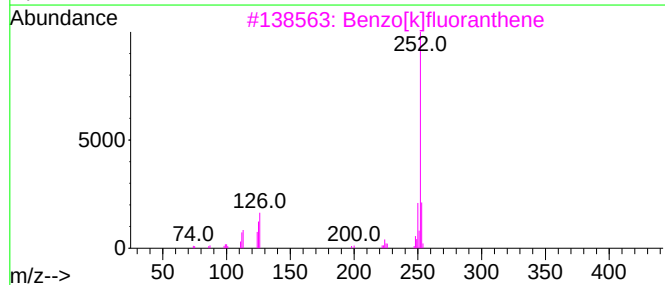
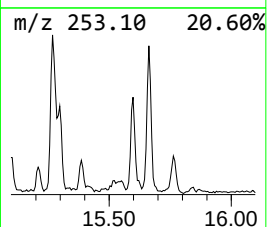
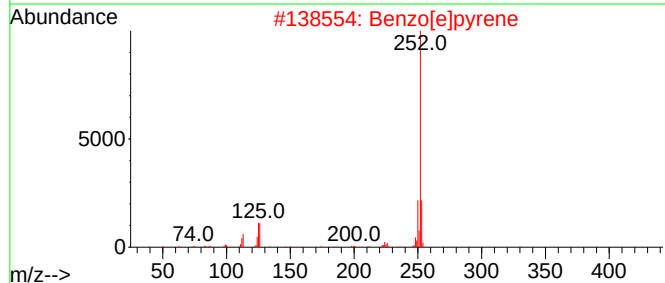
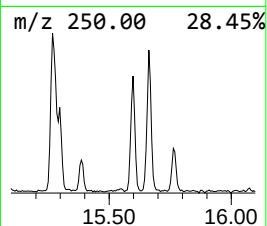
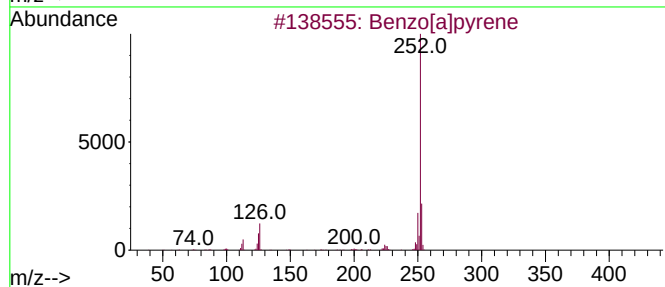
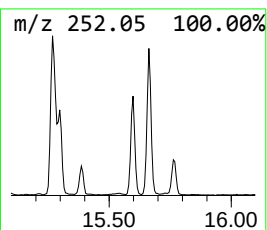
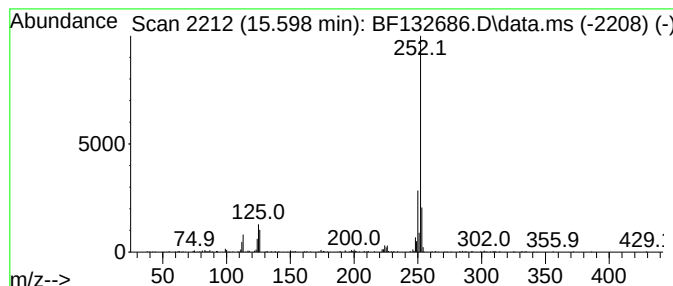
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.598	3.41 ng	180009	Perylene-d12	15.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030723\
Data File : BF132686.D
Acq On : 07 Mar 2023 19:38
Operator : CG\JU
Sample : 01825-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-TP4-0306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.228	32.3	ng	1787340	1	6.987	1108220	20.0
Benzophenone	10.745	2.3	ng	192122	3	10.034	1650080	20.0
n-Hexadecanoic ...	12.039	6.1	ng	534326	4	11.528	1757570	20.0
Biphenyl, 2,4,4...	12.669	3.2	ng	277324	4	11.528	1757570	20.0
Pentadecafluoro...	14.010	7.1	ng	509784	5	14.186	1436140	20.0
Squalene	15.039	10.6	ng	560786	6	15.733	1056600	20.0
Benzo[e]pyrene	15.598	3.4	ng	180009	6	15.733	1056600	20.0